

# Quantities and units

## Part 9: Physical chemistry and molecular physics

ICS 01.060

## National foreword

This British Standard is the UK implementation of EN ISO 80000-9:2013+A1:2011. It is identical to ISO 80000-9:2009, incorporating amendment 1:2011. It supersedes BS ISO 80000-9:2009, which is withdrawn.

The start and finish of text introduced or altered by amendment is indicated in the text by tags. Tags indicating changes to ISO text carry the number of the amendment. For example, text altered by ISO amendment 1 is indicated in the text by A1 A1.

The UK participation in its preparation was entrusted to Technical Committee SS/7, General metrology, quantities, units and symbols.

A list of organizations represented on this committee can be obtained on request to its secretary.

This publication does not purport to include all the necessary provisions of a contract. Users are responsible for its correct application.

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31 August 2011	Implementation of ISO amendment 1:2011
30 June 2013	This corrigendum renumbers BS ISO 80000-9:2009 as BS EN ISO 80000-9:2013

ICS 01.060

English Version

## Quantities and units - Part 9: Physical chemistry and molecular physics (ISO 80000-9:2009 + Amd 1:2011)

Grandeurs et unités - Partie 9: Chimie physique et physique moléculaire (ISO 80000-9:2009 + Amd 1:2011)

Größen und Einheiten - Teil 9: Physikalische Chemie und Molekularphysik (ISO 80000-9:2009 + Amd 1:2011)

This European Standard was approved by CEN on 14 March 2013.

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COMITÉ EUROPÉEN DE NORMALISATION  
EUROPÄISCHES KOMITEE FÜR NORMUNG

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## **Foreword**

The text of ISO 80000-9:2009 + Amd 1:2011 has been prepared by Technical Committee ISO/TC 12 “Quantities and units” of the International Organization for Standardization (ISO) and has been taken over as EN ISO 80000-9:2013.

This European Standard shall be given the status of a national standard, either by publication of an identical text or by endorsement, at the latest by October 2013, and conflicting national standards shall be withdrawn at the latest by October 2013.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. CEN [and/or CENELEC] shall not be held responsible for identifying any or all such patent rights.

According to the CEN-CENELEC Internal Regulations, the national standards organizations of the following countries are bound to implement this European Standard: Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Former Yugoslav Republic of Macedonia, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and the United Kingdom.

### **Endorsement notice**

The text of ISO 80000-9:2009 + Amd 1:2011 has been approved by CEN as EN ISO 80000-9:2013 without any modification.

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## Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 2.

The main task of technical committees is to prepare International Standards. Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

ISO 80000-9 was prepared by Technical Committee ISO/TC 12<sup>(A1)</sup> in collaboration with IEC/TC 25, *Quantities and units*.<sup>(A1)</sup>

This first edition of ISO 80000-9 cancels and replaces ISO 31-8:1992. It also incorporates the Amendment ISO 31-8:1992/Amd.1:1998. The major technical changes from the previous standard are the following:

- the presentation of *Numerical statements* has been changed;
- the *Normative references* have been changed;
- some new items have been introduced;
- some new chemical elements have been introduced in Annex A;
- Annex C on pH has been revised and given a completely new text.

ISO 80000 consists of the following parts, under the general title *Quantities and units*:

- *Part 1: General*
- *Part 2: Mathematical signs and symbols to be used in the natural sciences and technology*
- *Part 3: Space and time*
- *Part 4: Mechanics*
- *Part 5: Thermodynamics*
- *Part 7: Light*
- *Part 8: Acoustics*
- *Part 9: Physical chemistry and molecular physics*
- *Part 10: Atomic and nuclear physics*
- *Part 11: Characteristic numbers*
- *Part 12: Solid state physics*

IEC 80000 consists of the following parts, under the general title *Quantities and units*:

- *Part 6: Electromagnetism*
- *Part 13: Information science and technology*
- *Part 14: Telebiometrics related to human physiology*

## Introduction

### 0.1 Arrangements of the tables

The tables of quantities and units in this International Standard are arranged so that the quantities are presented on the left-hand pages and the units on the corresponding right-hand pages.

All units between two full lines on the right-hand pages belong to the quantities between the corresponding full lines on the left-hand pages.

Where the numbering of an item has been changed in the revision of a part of ISO 31, the number in the preceding edition is shown in parentheses on the left-hand page under the new number for the quantity; a dash is used to indicate that the item in question did not appear in the preceding edition.

### 0.2 Tables of quantities

The names in English and in French of the most important quantities within the field of this International Standard are given together with their symbols and, in most cases, their definitions. These names and symbols are recommendations. The definitions are given for identification of the quantities in the International System of Quantities (ISQ), listed on the left-hand pages of the table; they are not intended to be complete.

The scalar, vectorial or tensorial character of quantities is pointed out, especially when this is needed for the definitions.

In most cases only one name and only one symbol for the quantity are given; where two or more names or two or more symbols are given for one quantity and no special distinction is made, they are on an equal footing. When two types of italic letters exist (for example as with  $\vartheta$  and  $\theta$ ;  $\varphi$  and  $\phi$ ;  $a$  and  $\alpha$ ;  $g$  and  $g$ ) only one of these is given. This does not mean that the other is not equally acceptable. It is recommended that such variants should not be given different meanings. A symbol within parentheses implies that it is a reserve symbol, to be used when, in a particular context, the main symbol is in use with a different meaning.

In this English edition, the quantity names in French are printed in an italic font, and are preceded by *fr.* The gender of the French name is indicated by (m) for masculine and (f) for feminine, immediately after the noun in the French name.

### 0.3 Tables of units

#### 0.3.1 General

**A1** The names of units for the corresponding quantities are given together with the international symbols and the definitions. These unit names are language-dependent, but the symbols are international and the same in all languages. For further information, see the SI Brochure (8th edition 2006) from BIPM and ISO 80000-1. **A1**

The units are arranged in the following way:

- a) The coherent SI units are given first. The SI units have been adopted by the General Conference on Weights and Measures (Conférence Générale des Poids et Mesures, CGPM). The use of coherent SI units

**A1** Text deleted **A1**

is recommended; decimal multiples and submultiples formed with the SI prefixes are recommended, even though not explicitly mentioned.

- b) Some non-SI units are then given, being those accepted by the International Committee for Weights and Measures (Comité International des Poids et Mesures, CIPM), or by the International Organization of Legal Metrology (Organisation Internationale de Métrologie Légale, OIML), or by ISO and IEC, for use with the SI.

Such units are separated from the SI units in the item by use of a broken line between the SI units and the other units.

- c) Non-SI units currently accepted by the CIPM for use with the SI are given in small print (smaller than the text size) in the “Conversion factors and remarks” column.
- d) Non-SI units that are not recommended are given only in annexes in some parts of this International Standard. These annexes are informative, in the first place for the conversion factors, and are not integral parts of the standard. These deprecated units are arranged in two groups:
- 1) units in the CGS system with special names;
  - 2) units based on the foot, pound, second, and some other related units.
- e) Other non-SI units are given for information, especially regarding the conversion factors, in informative annexes in some parts of this International Standard.

### **0.3.2 Remark on units for quantities of dimension one, or dimensionless quantities**

The coherent unit for any quantity of dimension one, also called a dimensionless quantity, is the number one, symbol 1. When the value of such a quantity is expressed, the unit symbol 1 is generally not written out explicitly.

EXAMPLE 1 Refractive index  $n = 1,53 \times 1 = 1,53$

Prefixes shall not be used to form multiples or submultiples of this unit. Instead of prefixes, powers of 10 are recommended.

EXAMPLE 2 Reynolds number  $Re = 1,32 \times 10^3$

Considering that plane angle is generally expressed as the ratio of two lengths and solid angle as the ratio of two areas, in 1995 the CGPM specified that, in the SI, the radian, symbol rad, and steradian, symbol sr, are dimensionless derived units. This implies that the quantities plane angle and solid angle are considered as derived quantities of dimension one. The units radian and steradian are thus equal to one; they may either be omitted, or they may be used in expressions for derived units to facilitate distinction between quantities of different kinds but having the same dimension.

## **0.4 Numerical statements in this International Standard**

The sign = is used to denote “is exactly equal to”, the sign  $\approx$  is used to denote “is approximately equal to”, and the sign := is used to denote “is by definition equal to”.

Numerical values of physical quantities that have been experimentally determined always have an associated measurement uncertainty. This uncertainty should always be specified. In this International Standard, the magnitude of the uncertainty is represented as in the following example.

EXAMPLE  $l = 2,347\ 82(32)\ \text{m}$

In this example,  $l = a(b)\ \text{m}$ , the numerical value of the uncertainty  $b$  indicated in parentheses is assumed to apply to the last (and least significant) digits of the numerical value  $a$  of the length  $l$ . This notation is used when  $b$  represents one standard uncertainty (estimated standard deviation) in the last digits of  $a$ . The numerical example given above may be interpreted to mean that the best estimate of the numerical value of the length  $l$  (when  $l$  is expressed in the unit metre) is 2,347 82, and that the unknown value of  $l$  is believed to lie between  $(2,347\ 82 - 0,000\ 32)\ \text{m}$  and  $(2,347\ 82 + 0,000\ 32)\ \text{m}$  with a probability determined by the standard uncertainty 0,000 32 m and the probability distribution of the values of  $l$ .



## 0.5 Special remarks

In this part of ISO 80000, symbols for substances are shown as subscripts, for example  $c_B$ ,  $w_B$ ,  $p_B$ .

Generally, it is advisable to put symbols for substances and their states in parentheses on the same line as the main symbol, for example  $c(\text{H}_2\text{SO}_4)$ .

The superscript \* is used to mean "pure". The superscript  $\ominus$  is used to mean "standard".

EXAMPLE 1  $V_m(\text{K}_2\text{SO}_4, 0,1 \text{ mol} \cdot \text{dm}^{-3} \text{ in } \text{H}_2\text{O}, 25 \text{ }^\circ\text{C})$  for molar volume.

EXAMPLE 2  $C_{m,p}^\ominus(\text{H}_2\text{O}, \text{g}, 298,15 \text{ K}) = 33,58 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  for standard molar heat capacity at constant pressure.

In an expression such as  $\varphi_B = x_B V_{m,B}^* / \sum x_i V_{m,i}^*$ , where  $\varphi_B$  denotes the volume fraction of a particular substance B in a mixture of substances A, B, C, ..., where  $x_i$  denotes the amount-of-substance fraction of  $i$  and  $V_{m,i}^*$  the molar volume of the pure substance  $i$ , and where all the molar volumes  $V_{m,A}^*$ ,  $V_{m,B}^*$ ,  $V_{m,C}^*$ , ... are taken at the same temperature and pressure, the summation on the right-hand side is that over all the substances A, B, C, ... of which a mixture is composed, so that  $\sum x_i = 1$ .

The names and symbols of the chemical elements are given in Annex A.

Additional qualifying information on a quantity symbol may be added as a subscript or superscript or in parentheses after the symbol.



# Quantities and units —

## Part 9: Physical chemistry and molecular physics

### 1 Scope

ISO 80000-9 gives names, symbols, and definitions for quantities and units of physical chemistry and molecular physics. Where appropriate, conversion factors are also given.

### 2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 80000-3:2006, *Quantities and units — Part 3: Space and time*

ISO 80000-4:2006, *Quantities and units — Part 4: Mechanics*

ISO 80000-5:2007, *Quantities and units — Part 5: Thermodynamics*

IEC 80000-6:2008, *Quantities and units — Part 6: Electromagnetism*

### 3 Names, symbols, and definitions

The names, symbols, and definitions for quantities and units of physical chemistry and molecular physics are given on the following pages.

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS			QUANTITIES	
Item No.	Name	Symbol	Definition	Remarks
9-1 (8-3)	amount of substance <i>fr quantité (f) de matière</i>	$n$	amount of substance is one of the seven base quantities in the International System of Quantities, ISQ, on which the SI is based	<p>Amount of substance of a pure sample is that quantity that can often be determined by measuring its mass and dividing by the molar mass of the sample.</p> <p>Amount of substance is defined to be proportional to the number of specified elementary entities in a sample, the proportionality constant being a universal constant which is the same for all samples.</p> <p>The name “number of moles” is often used for “amount of substance”, but this is deprecated because the name of a quantity should be distinguished from the name of the unit.</p> <p>In the name “amount of substance”, the words “of substance” could, for simplicity, be replaced by words to specify the substance concerned in any particular application, so that one may, for example, talk of “amount of hydrogen chloride, HCl”, or “amount of benzene, C<sub>6</sub>H<sub>6</sub>”.</p> <p>It is important to always give a precise specification of the entity involved (as emphasized in the second sentence of the definition of the mole); this should preferably be done by giving the molecular chemical formula of the material involved.</p>

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-1.a	mole	mol	<p>the mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0,012 kg of carbon 12</p> <p>[14th CGPM (1971)]</p>	<p>When the mole is used, the elementary entities shall be specified and may be atoms, molecules, ions, electrons, other entities or specified groups of them.</p> <p>The definition applies to unbound atoms of carbon 12, at rest and in their ground state.</p> <p>The mole is also used for entities such as holes and other quasi-particles, double bonds, etc.</p>

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-2.1 (8-1.1)	relative atomic mass <i>fr masse (f) atomique relative</i>	$A_r$	ratio of the average mass (ISO 80000-4:2006, item 4-1) per atom of an element to 1/12 of the mass of an atom of the nuclide $^{12}\text{C}$	EXAMPLE $A_r(\text{Cl}) \approx 35,453$ The relative atomic or relative molecular mass depends on the nuclidic composition.
9-2.2 (8-1.2)	relative molecular mass <i>fr masse (f) moléculaire relative</i>	$M_r$	ratio of the average mass per molecule or specified entity of a substance to 1/12 of the mass of an atom of the nuclide $^{12}\text{C}$	The International Union of Pure and Applied Chemistry (IUPAC) accepts the use of the special names “atomic weight” and “molecular weight” for the quantities “relative atomic mass” and “relative molecular mass”, respectively. The use of these traditional names is deprecated.
9-3 (8-2)	number of particles <i>fr nombre (m) de particules</i>	$N_B$	$N_B$ equals the number of particles in a system	Different entities may be used as a particle, e.g. number of molecules, number of atoms. A subscript added to the symbol indicates a specific entity, e.g. $N_B$ for the number of molecules of substance B.
9-4 (8-4)	Avogadro constant <i>fr constante (f) d'Avogadro</i>	$L, N_A$	for a pure sample $L = N/n$ where $N$ is the number of particles (item 9-3) and $n$ is amount of substance (item 9-1)	$L = 6,022\,141\,79(30) \times 10^{23} \text{ mol}^{-1}$ [A1] [CODATA 2006]
9-5 (8-5)	molar mass <i>fr masse (f) molaire</i>	$M$	for a pure sample $M = m/n$ where $m$ is mass (ISO 80000-4:2006, item 4-1) and $n$ is amount of substance (item 9-1)	
9-6 (8-6)	molar volume <i>fr volume (m) molaire</i>	$V_m$	for a pure sample $V_m = V/n$ where $V$ is volume (ISO 80000-3:2006, item 3-4) and $n$ is amount of substance (item 9-1)	The molar volume of an ideal gas at 273,15 K and 101 325 Pa is $V_m = 0,022\,413\,996\,(39) \text{ m}^3/\text{mol}$ and, for 273,15 K and 100 000 Pa, the molar volume is $V_m = 0,022\,710\,981\,(40) \text{ m}^3/\text{mol}$ . [CODATA 2006]

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-2.a	one	1		See the Introduction, 0.3.2.
9-3.a	one	1		See the Introduction, 0.3.2.
9-4.a	mole to the power minus one	mol <sup>-1</sup>		
9-5.a	kilogram per mole	kg/mol		The commonly used unit for molar mass is gram per mole, g/mol, rather than kilogram per mole, kg/mol.
9-6.a	cubic metre per mole	m <sup>3</sup> /mol		

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-7 (8-7)	molar internal energy <i>fr énergie (f) interne molaire</i>	$U_m$	$U_m = U/n$ where $U$ is internal energy (ISO 80000-5:2007, item 5-20.2) and $n$ is amount of substance (item 9-1)	Similar definitions apply to other thermodynamic functions, for example molar enthalpy, $H_m$ , molar Helmholtz energy, $A_m$ , and molar Gibbs energy, $G_m$ . These quantities are normally only used with reference to pure substances. Molar heat capacity may be defined at constant pressure, $C_{m,p}$ or at constant volume, $C_{m,v}$ .
9-8 (8-8)	molar heat capacity <i>fr capacité (f) thermique molaire</i>	$C_m$	$C_m = C/n$ where $C$ is heat capacity (ISO 80000-5:2007, item 5-15) and $n$ is amount of substance (item 9-1)	
9-9 (8-9)	molar entropy <i>fr entropie (f) molaire</i>	$S_m$	$S_m = S/n$ where $S$ is entropy (ISO 80000-5:2007, item 5-18) and $n$ is amount of substance (item 9-1)	
9-10.1 (8-10.1)	volumic number of molecules or other elementary entities, number density of molecules or other elementary entities <i>fr nombre (m) volumique de molécules ou d'autres entités élémentaires</i>	$n, (C)$	$n = N/V$ where $N$ is the number of particles (item 9-3) and $V$ is volume (ISO 80000-3:2006, item 3-4)	
9-10.2 (8-10.2)	molecular concentration of substance B <i>fr concentration (f) moléculaire du constituant B</i>	$C_B$	$C_B = N_B/V$ where $N_B$ is the number of molecules of B and $V$ is the volume (ISO 80000-3:2006, item 3-4) of the mixture	



UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-7.a	joule per mole	J/mol		
9-8.a	joule per mole kelvin	J/(mol · K)		
9-9.a	joule per mole kelvin	J/(mol · K)		
9-10.a	metre to the power minus three	m <sup>-3</sup>		

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-11.1 (8-11.1)	mass density, density <i>fr masse (f) volumique</i>	$\rho, (\gamma)$	$\rho = m/V$ where $m$ is mass (ISO 80000-4:2006, item 4-1) and $V$ is volume (ISO 80000-3:2006, item 3-4)	
9-11.2 (8-11.2)	mass concentration of substance B <i>fr concentration (f) en masse du constituant B</i>	$\rho_B, (\gamma_B)$	$\rho_B = m_B/V$ where $m_B$ is the mass (ISO 80000-4:2006, item 4-1) of substance B and $V$ is the volume (ISO 80000-3:2006, item 3-4) of the mixture	
9-12 (8-12)	mass fraction of substance B <i>fr fraction (f) massique du constituant B</i>	$w_B$	$w_B = m_B/m$ where $m_B$ is the mass (ISO 80000-4:2006, item 4-1) of substance B and $m$ is the total mass of the mixture	
9-13 (8-13)	amount-of- substance concentration of B <i>fr concentration (f) en quantité de matière du constituant B</i>	$c_B$	$c_B = n_B/V$ where $n_B$ is the amount of substance (item 9-1) of B and $V$ is the volume (ISO 80000-3:2006, item 3-4) of the solution	In chemistry, the name “amount-of-substance concentration” is generally abbreviated to the single word “concentration”, it being assumed that the adjective “amount-of-substance” is intended. For this reason, however, the word “mass” should never be omitted from the name “mass concentration” in 9-11.2.  The standard concentration, 1 mol/dm <sup>3</sup> , is denoted $c^{-e}$ .
9-14 (8-14.1)	amount-of- substance fraction of B, (mole fraction of substance B) <i>fr fraction (f) molaire du constituant B</i>	$x_B, y_B$	$x_B = n_B/n$ where $n_B$ is the amount of substance (item 9-1) of B and $n$ is the total amount of substance (item 9-1) in the mixture	For condensed phases, $x_B$ is used, and for gaseous mixtures $y_B$ may be used.  The unsystematic name “mole fraction” is still used. However, the use of this name is deprecated.  For this quantity, the entity used to define the amount of substance should always be a single molecule for every species in the mixture.

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-11.a	kilogram per cubic metre	kg/m <sup>3</sup>		
9-11.b	gram per litre	g/l		1 g/l = 1 g/dm <sup>3</sup> = 1 kg/m <sup>3</sup>
9-12.a	one	1		See the Introduction, 0.3.2.
9-13.a	mole per cubic metre	mol/m <sup>3</sup>		
9-13.b	mole per litre	mol/l		1 mol/l = 1 mol/dm <sup>3</sup> = 10 <sup>3</sup> mol/m <sup>3</sup>
9-14.a	one	1		See the Introduction, 0.3.2.

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-15 (8-15)	volume fraction of substance B <i>fr fraction (f) volumique du constituant B</i>	$\varphi_B$	$\varphi_B = \frac{x_B V_{m,B}^*}{\sum x_i V_{m,i}^*}$ <p>where the <math>V_{m,i}^*</math> is the molar volume (item 9-6) of the pure substances <math>i</math> at the same temperature and pressure, <math>x_i</math> denotes the amount-of-substance fraction (item 9-14) of substance <math>i</math> and <math>\Sigma</math> denotes summation over all substances <math>i</math></p>	$\varphi_B$ is temperature-dependent.
9-16 (8-16)	molality of solute B <i>fr molalité (f) du soluté B</i>	$b_B, m_B$	$b_B = n_B/m_A$ <p>where <math>n_B</math> is the amount of substance (item 9-1) of solute B and <math>m_A</math> is the mass (ISO 80000-4:2006, item 4-1) of the solvent substance A</p>	The alternative symbol $m_B$ should be avoided in situations where it might be mistaken for the mass of substance B.  However, the symbol $m$ is much more commonly used than the symbol $b$ for molality, despite the possible confusion with mass.
9-17 (8-17)	chemical potential of substance B <i>fr potentiel (m) chimique du constituant B</i>	$\mu_B$	for a mixture of substances $i$ $\mu_B = (\partial G/\partial n_B)_{T,p,n_i}$ <p>where <math>G</math> is Gibbs energy (ISO 80000-5:2007, item 5-20.5) and <math>n_B</math> is the amount of substance B (item 9-1)</p>	For a pure substance, $\mu = G/n = G_m$ <p>where <math>G_m</math> is the molar Gibbs energy. In a mixture, <math>\mu_B</math> is the partial molar Gibbs energy.</p>
9-18 (8-18)	absolute activity of substance B <i>fr activité (f) absolue du constituant B</i>	$\lambda_B$	$\lambda_B = \exp(\mu_B/RT)$ <p>where <math>\mu_B</math> is the chemical potential of substance B (item 9-17), <math>R</math> is the molar gas constant (item 9-42), and <math>T</math> is thermodynamic temperature (ISO 80000-5:2007, item 5-1)</p>	
9-19 (8-19)	partial pressure of substance B <i>fr pression (f) partielle du constituant B</i>	$p_B$	for a gaseous mixture, $p_B = x_B \cdot p$ <p>where <math>x_B</math> is the amount-of-substance fraction of substance B (item 9-14) and <math>p</math> is the total pressure (ISO 80000-4:2006, item 4-15.1)</p>	

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-15.a	one	1		See the Introduction, 0.3.2.
9-16.a	mole per kilogram	mol/kg		
9-17.a	joule per mole	J/mol		
9-18.a	one	1		See the Introduction, 0.3.2.
9-19.a	pascal	Pa		

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-20 (8-20)	fugacity of substance B in a gaseous mixture <i>fr fugacité (f) du constituant B dans un mélange gazeux</i>	$\tilde{p}_B, (f_B)$	for a gaseous mixture, $\tilde{p}_B$ is proportional to the absolute activity, $\lambda_B$ (item 9-18), the proportionality factor, which is a function of temperature only, being determined by the condition that, at constant temperature and composition, $p_B/\tilde{p}_B$ tends to 1 for an indefinitely dilute gas	$\tilde{p}_B = \lambda_B \cdot \lim_{p \rightarrow 0} (p_B/\lambda_B)$ where $p$ is total pressure.
9-21 (—)	standard chemical potential of substance B <i>fr potentiel (m) chimique de référence du constituant B</i>	$\mu_B^\ominus$	value of the chemical potential (item 9-17) at standard conditions	$\mu^\ominus = RT \ln \lambda^\ominus$ $\mu_B^\ominus$ is a function of temperature $T$ at the standard pressure $p = p^\ominus$ . The standard chemical potential depends on the choice of standard state, which shall be specified.
9-22.1 (—)	standard chemical potential of substance B in a pure phase or a mixture or a solvent <i>fr potentiel (m) chimique de référence du constituant B dans une phase pure, un mélange ou un solvant</i>	$\mu_B^\ominus$	for a pure phase, or a mixture, or a solvent, the chemical potential (item 9-17) of the pure substance B under standard pressure	The plimsoll sign is used to denote a standard in general. The degree sign can also be used for this. In a liquid or solid solution, the standard state is referenced to the ideal dilute behaviour of the solute (substance B).
9-22.2 (—)	standard chemical potential of substance B in a solution <i>fr potentiel (m) chimique de référence du constituant B dans une solution</i>	$\mu_B^\ominus$	for a solute in solution, the chemical potential, $\mu_B^\ominus$ in the (hypothetical) state of solute B at the standard molality, $b^\ominus$ (item 9-16), and standard pressure, $p^\ominus$ (ISO 80000-4:2006, item 4-15.1), and behaving like an infinitely dilute solution: $\mu_B^\ominus = \lim_{p \rightarrow 0} \mu_B - RT \ln(y_B p/p^\ominus)$ where $y_B$ is amount-of-substance fraction (item 9-14)	

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-20.a	pascal	Pa		
9-21.a	joule per mole	J/mol		
9.22.a	joule per mole	J/mol		

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS			QUANTITIES	
Item No.	Name	Symbol	Definition	Remarks
9-23 (8-22.1)	activity factor of substance B in a liquid or a solid mixture activity coefficient of substance B in a liquid or a solid mixture <i>fr facteur (m)</i> <i>d'activité du constituant B dans un mélange liquide ou solide</i>	$f_B$	$f_B = \lambda_B / (\lambda_B^* x_B)$ where $\lambda_B$ is the absolute activity of substance B (item 9-18), $\lambda_B^*$ is the absolute activity of the pure substance B at the same temperature and pressure, and $x_B$ is the amount-of-substance fraction of substance B (item 9-14)	The systematic name is "activity factor", but the name "activity coefficient" is also commonly used.
9-24.1 (—)	activity factor referenced to Raoult's law <i>fr facteur (m)</i> <i>d'activité référencé à la loi de Raoult</i>	$f_B$	$f_B = a_B / x_B$ where $a_B$ is the activity of solute B (item 9-26) and $x_B$ is the amount-of-substance fraction of B (item 9-14)	
9-24.2 (—)	activity factor referenced to Henry's law <i>fr facteur (m)</i> <i>d'activité référencé à la loi de Henry</i>	$\gamma_m, \gamma_c, \gamma_x$	There are three different cases for the activity factor referenced to Henry's law: molality basis, $\gamma_m$ , concentration basis, $\gamma_c$ , and amount-of-substance basis, $\gamma_x$ : $\gamma_{m,B} = \frac{a_{m,B}}{b_B / b^\ominus}$ $\gamma_{c,B} = \frac{a_{c,B}}{c_B / c^\ominus}$ $\gamma_{x,B} = \frac{a_{x,B}}{x_B}$	
9-25 (8-22.2)	standard absolute activity of substance B in a liquid or a solid mixture <i>fr activité (f)</i> <i>absolue normale du constituant B dans un mélange liquide ou solide</i>	$\lambda_B^\ominus$	$\lambda_B^\ominus = \lambda_B^* (p^\ominus)$ where $\lambda_B^*$ is the absolute activity (item 9-18) of the pure substance B at the same temperature and pressure, and $p^\ominus$ is standard pressure (ISO 80000-4:2006, item 4-15.1)	This quantity is a function of temperature only. The standard pressure is $10^5$ Pa.



UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-23.a	one	1		See the Introduction, 0.3.2.
9-24.a	one	1		See the Introduction, 0.3.2.
9-25.a	one	1		See the Introduction, 0.3.2.

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-26 (8-23)	activity of solute B, relative activity of solute B <i>fr activité (f) du soluté B, activité (f) relative du soluté B</i>	$a_B, a_{m,B}$	for a solute B in a solution, $a_B$ is proportional to the absolute activity, $\lambda_B$ (item 9-18), the proportionality factor, which is a function of temperature and pressure only, being determined by the condition that, at constant temperature and pressure, $a_B$ divided by the molality ratio, $b_B/b^\ominus$ , tends to 1 at infinite dilution; $b_B$ is the molality of solute B (item 9-16), and $b^\ominus$ is standard molality, usually 1 mol/kg	$a_B = \lambda_B \cdot \lim_{b_B \rightarrow 0} \frac{b_B/b^\ominus}{\lambda_B}$ <p>The quantity <math>a_{c,B}</math>, similarly defined in terms of the concentration ratio <math>c_B/c^\ominus</math>, is also called the activity or relative activity of solute B; <math>c^\ominus</math> is a standard concentration, usually 1 mol/dm<sup>3</sup>:</p> $a_{c,B} = \lambda_B \cdot \lim_{c_B \rightarrow 0} \frac{c_B/c^\ominus}{\lambda_B}$ <p>where <math>\Sigma</math> denotes summation over all the solute substances. This especially applies to a dilute liquid solution.</p>
9-27 (8-24.1)	activity coefficient of solute B <i>fr facteur (m) d'activité du soluté B</i>	$\gamma_B$	for a solute in a solution, $\gamma_B = \frac{a_B}{b_B/b^\ominus}$ where $a_B$ is the activity of solute B (item 9-26), $b_B$ is the molality of substance B, and $b^\ominus$ is standard molality	The name "activity coefficient of solute B" is also used for the quantity $\gamma_B$ defined as $\gamma_B = \frac{a_{c,B}}{c_B/c^\ominus}$ See item 9-26.
9-28 (8-24.2)	standard absolute activity of solute B <i>fr activité (f) absolue normale du soluté B</i>	$\lambda_B^\ominus$	for a solute B in a solution, $\lambda_B^\ominus = \lim_{b_B \rightarrow 0} [\lambda_B (p^\ominus) b^\ominus / b_B]$ where $\Sigma$ denotes summation over all solutes, $p^\ominus$ is a standard pressure (ISO 80000-4:2006, item 4-15.1), $b^\ominus$ is standard molality, and $b_B$ is the molality of substance B (item 9-16)	This quantity is a function of temperature only. It especially applies to a dilute liquid solution. The standard pressure is 10 <sup>5</sup> Pa.

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-26.a	one	1		See the Introduction, 0.3.2.
9-27.a	one	1		See the Introduction, 0.3.2.
9-28.a	one	1		See the Introduction, 0.3.2.

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS			QUANTITIES	
Item No.	Name	Symbol	Definition	Remarks
9-29.1 (8-25.1)	activity of solvent A, relative activity of solvent A <i>fr activité (f) du solvant A, activité (f) relative du solvant A</i>	$a_A$	for the solvent A in a solution, ratio of the absolute activity of substance A, $\lambda_A$ (item 9-18), to that, $\lambda_A^*$ , of the pure solvent at the same temperature and pressure	$a_A = \lambda_A / \lambda_A^*$
9-29.2 (8-25.2)	osmotic factor of solvent A, osmotic coefficient of solvent A <i>fr facteur (m) osmotique du solvant A</i>	$\varphi$	$\varphi = - (M_A \sum b_B)^{-1} \ln a_A$ where $M_A$ is the molar mass (item 9-5) of the solvent A, $\sum$ denotes summation over all the solutes, $b_B$ is the molality of solute B (item 9-16), and $a_A$ is the activity of solvent A (item 9-29.1)	The name "osmotic coefficient" is generally used, although the name "osmotic factor" is more systematic. This especially applies to a dilute liquid solution.
9-29.3 (8-25.3)	standard absolute activity of solvent A (especially in a dilute liquid solution) <i>fr activité (f) absolue normale du solvant A (particulière- ment en solution liquide diluée)</i>	$\lambda_A^\ominus$	for the solvent A in a solution, the absolute activity (item 9-18) of the pure substance A at the same temperature and at a standard pressure $p^\ominus$ (ISO 80000-4:2006, item 4-15.1):  $\lambda_A^\ominus = \lambda_A^* p^\ominus$	The standard pressure is $10^5$ Pa.
9-30 (8-26)	osmotic pressure <i>fr pression (f) osmotique</i>	$\Pi$	excess pressure required to maintain osmotic equilibrium between a solution and the pure solvent separated by a membrane permeable to the solvent only	
9-31 (8-27)	stoichiometric number of substance B <i>fr nombre (m) stœchio- métrique du constituant B</i>	$\nu_B$	number or simple fraction occurring in the expression for a chemical reaction: $0 = \sum \nu_B B$ , where the symbol B denotes the reactants and products involved in the reaction	EXAMPLE $(1/2)\text{N}_2 + (3/2)\text{H}_2 = \text{NH}_3$ $\nu(\text{N}_2) = -1/2,$ $\nu(\text{H}_2) = -3/2,$ $\nu(\text{NH}_3) = +1.$  The stoichiometric number is negative for a reactant and positive for a product.

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-29.a	one	1		See the Introduction, 0.3.2.
9-30.a	pascal	Pa		
9-31.a	one	1		See the Introduction, 0.3.2.

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-32 (8-28)	affinity of a chemical reaction <i>fr affinité (f) d'une réaction chimique</i>	$A$	$A = -\sum \nu_B \mu_B$ where $\nu_B$ is the stoichiometric number of substance B (item 9-31) and $\mu_B$ is the chemical potential of substance B (item 9-17)  The summation goes over all substances B.	The affinity of a reaction is a measure of the "driving force" of the reaction. When it is positive, the reaction goes spontaneously from reactants to products, and when it is negative, the reaction goes in the opposite direction.  Another way to write the definition is: $A = -(\partial G / \partial \xi)_{p,T}$ where $G$ is Gibbs energy (ISO 80000-5:2007, item 5-20.5) and $\xi$ is the extent of the reaction (item 9-33).  Note that $\nu_B$ is negative for reactants and positive for products.
9-33 (8-29)	extent of reaction <i>fr état (m) d'avancement d'une réaction</i>	$\xi$	$dn_B = \nu_B d\xi$ where $n_B$ is the amount of substance B (item 9-1) and $\nu_B$ is the stoichiometric number of substance B (item 9-31)	See remark to item 9-31.
9-34 (8-30)	standard equilibrium constant, thermodynamic equilibrium constant <i>fr constante (f) d'équilibre normale</i>	$K^\ominus$	for a chemical reaction, $K^\ominus = \prod_B (\lambda_B^\ominus)^{-\nu_B}$ where $\prod_B$ denotes the product for all substances B, $\lambda_B^\ominus$ is the standard absolute activity of substance B (item 9-25) and $\nu_B$ is the stoichiometric number of substance B (item 9-31)	This quantity is a function of temperature only.  Others depend on temperature, pressure, and composition, as follows.  One can define in an analogous way an equilibrium constant in terms of fugacity, $K_f$ , molality, $K_m$ , etc.
9-35	equilibrium constant on a pressure basis <i>fr constante (f) d'équilibre pour les pressions</i>	$K_p$	$K_p = \prod_B (p_B)^{\nu_B}$ for gases	

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-32.a	joule per mole	J/mol		
9-33.a	mole	mol		
9-34.a	one	1		See the Introduction, 0.3.2.
9-35.a	pascal to the power sum of stoichiometric numbers	$\text{Pa}^{\sum \nu_B}$		

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-36	equilibrium constant on a concentration basis <i>fr constante (f) d'équilibre pour les concentrations</i>	$K_c$	$K_c = \prod_B (c_B)^{\nu_B}$ for solutions	
9-37 (8-32)	electric dipole moment of a molecule <i>fr moment (m) électrique d'une molécule</i>	$\mathbf{p}, (\mu)$	$E_p = -\mathbf{p} \cdot \mathbf{E}$ where $E_p$ is the interaction energy (ISO 80000-5:2007, item 5-20.1) of the molecule with electric dipole moment $\mathbf{p}$ and an electric field with electric field strength $\mathbf{E}$ (IEC 80000-6:2008, item 6-10)	The moment of force $\mathbf{M}$ acting in an electric field $\mathbf{E}$ on a neutral system with dipole moment $\mathbf{p}$ is given by $\mathbf{M} = \mathbf{p} \times \mathbf{E}$ .
9-38 (—)	magnetic dipole moment of a molecule <i>fr moment (m) magnétique d'une molécule</i>	$\mathbf{m}, \mu$	$E_m = -\mathbf{m} \cdot \mathbf{B}$ where $E_m$ is the interaction energy (ISO 80000-5:2007, item 5-20.1) of the molecule with magnetic dipole moment $\mathbf{m}$ and a magnetic field with magnetic flux density $\mathbf{B}$ (IEC 80000-6:2008, item 6-21)	The moment of force $\mathbf{M}$ acting in a magnetic flux density $\mathbf{B}$ on a neutral system with dipole moment $\mathbf{m}$ is given by $\mathbf{M} = \mathbf{m} \times \mathbf{B}$ .
9-39 (8-33)	electric polarizability of a molecule <i>fr polarisabilité (f) électrique d'une molécule</i>	$\alpha$	$\alpha_{ij} = \partial p_i / \partial E_j$ where $p_i$ is the cartesian component along the $i$ -axis of the electric dipole moment (item 9-37) induced by the applied electric field strength (IEC 80000-6:2008, item 6-10) acting on the molecule, and $E_j$ is the component along the $j$ -axis of this electric field strength	



UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-36.a	mole per cubic metre to the power sum of stoichiometric numbers	$(\text{mol} \cdot \text{m}^{-3})^{\sum \nu_B}$		
9-37.a	coulomb metre	C · m		
9-38.a	joule per tesla ampere metre squared	J/T A · m <sup>2</sup>		
9-39.a	coulomb metre squared per volt	C · m <sup>2</sup> /V		

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-40.1 (8-34.1)	microcanonical partition function <i>fr fonction (f) de partition micro-canonique</i>	$\Omega$	$\Omega = \sum_r 1$ where the sum is over all quantum states consistent with given energy, volume, external fields, and content	$S = k \ln \Omega$ where $S$ is the entropy (ISO 80000-5:2007, item 5-18) and $k$ is the Boltzmann constant (item 9-43).
9-40.2 (8-34.2)	canonical partition function <i>fr fonction (f) de partition canonique</i>	$Z, Q$	$Z = \sum_r e^{-E_r/kT}$ where the sum is over all quantum states consistent with given energy, volume, external fields, and content, $E_r$ is the energy (ISO 80000-5:2007, item 5-20.1) in the $r$ th quantum state, $k$ is the Boltzmann constant (item 9-43), and $T$ is thermodynamic temperature (ISO 80000-5:2007, item 5-1)	$A = -kT \ln Z$ where $A$ is the Helmholtz free energy (ISO 80000-5:2007, item 5-20.4).
9-40.3 (8-34.3)	grand-canonical partition function, grand partition function <i>fr fonction (f) de partition grand-canonique</i>	$\Xi$	$\Xi = \sum_{N_A, N_B, \dots} Z(N_A, N_B, \dots) \cdot \lambda_A^{N_A} \cdot \lambda_B^{N_B} \cdot \dots$ where $Z(N_A, N_B, \dots)$ is the canonical partition function for the given number of particles A, B, ..., and $\lambda_A, \lambda_B, \dots$ are the absolute activities of particles A, B, ...	$A - \sum \mu_B n_B = -kT \ln \Xi$ where $\mu_B$ is the chemical potential of substance B, $n_B$ is the amount of substance B, $k$ is the Boltzmann constant, and $T$ is thermodynamic temperature.
9-40.4 (8-34.4)	molecular partition function, partition function of a molecule <i>fr fonction (f) de partition moléculaire</i>	$q$	$q = \sum_i \exp(-\varepsilon_i/kT)$ where $\varepsilon_i$ is the energy (ISO 80000-5:2007, item 5-20.1) of the $i$ th allowed quantum state of the molecule consistent with given volume and external fields, $k$ is the Boltzmann constant (item 9-43), and $T$ is thermodynamic temperature (ISO 80000-5:2007, item 5-1)	
9-41 (8-35)	statistical weight <i>fr poids (m) statistique</i>	$g$	multiplicity of quantum energy levels	Multiplicity is also known as "degeneracy".
9-42 (8-36)	molar gas constant <i>fr constante (f) molaire des gaz</i>	$R$	for an ideal gas, $pV_m = RT$ where $p$ is pressure (ISO 80000-4:2006, item 4-15.1), $V_m$ is molar volume (item 9-6), and $T$ is thermodynamic temperature (ISO 80000-5:2007, item 5-1)	$R = 8,314\,472\,(15)\text{ J}/(\text{mol} \cdot \text{K})$ [CODATA 2006]

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-40.a	one	1		See the Introduction, 0.3.2.
9-41.a	one	1		See the Introduction, 0.3.2.
9-42.a	joule per mole kelvin	J/(mol·K)		

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-43 (8-37)	Boltzmann constant <i>fr constante (f) de Boltzmann</i>	$k$	$k = R/N_A$ where $R$ is the molar gas constant (item 9-42) and $N_A$ is the Avogadro constant (item 9-4)	$k = 1,380\,650\,4\,(24) \times 10^{-23}$ J/K [CODATA 2006]
9-44 (8-38)	mean free path <i>fr libre parcours (m) moyen</i>	$l, \lambda$	for a particle, the average distance between two successive collisions with other molecules	
9-45 (8-39)	diffusion coefficient <i>fr coefficient (m) de diffusion</i>	$D$	$C_B \langle v_B \rangle = -D \mathbf{grad} C_B$ where $C_B$ is the local molecular concentration of substance B (item 9-10.2) in the mixture and $\langle v_B \rangle$ is the local average velocity (ISO 80000-3:2006, item 3-8.1) of the molecules of B	
9-46.1 (8-40.1)	thermal diffusion ratio <i>fr rapport (m) de diffusion thermique</i>	$k_T$	in a steady state of a binary mixture in which thermal diffusion occurs, $\mathbf{grad} x_B = -(k_T/T) \mathbf{grad} T$ where $x_B$ is the amount-of-substance fraction (item 9-14) of the heavier substance B, and $T$ is the local thermodynamic temperature (ISO 80000-5:2007, item 5-1)	
9-46.2 (8-40.2)	thermal diffusion factor <i>fr facteur (m) de diffusion thermique</i>	$\alpha_T$	$\alpha_T = k_T/(x_A x_B)$ where $k_T$ is the thermal diffusion ratio (item 9-46.1), and $x_A$ and $x_B$ are the local amount-of-substance fractions (item 9-14) of the two substances A and B	
9-47 (8-41)	thermal diffusion coefficient <i>fr coefficient (m) de diffusion thermique</i>	$D_T$	$D_T = k_T \cdot D$ where $k_T$ is the thermal diffusion ratio (item 9-46.1) and $D$ is the diffusion coefficient (item 9-45)	
9-48 (8-42)	proton number, atomic number <i>fr nombre (m) de protons, numéro (m) atomique</i>	$Z$	number of protons in an atomic nucleus	The atomic number in the periodic table is equal to the proton number.

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-43.a	joule per kelvin	J/K		
9-44.a	metre	m		
9-45.a	metre squared per second	m <sup>2</sup> /s		
9-46.a	one	1		See the Introduction, 0.3.2.
9-47.a	metre squared per second	m <sup>2</sup> /s		
9-48.a	one	1		See the Introduction, 0.3.2.

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-49 (8-43)	elementary charge <i>fr charge (f) élémentaire</i>	$e$	electric charge (IEC 80000-6:2008, item 6-2) of a proton	$e = 1,602\ 176\ 487(40) \times 10^{-19}\ \text{C}$ [CODATA 2006] The electric charge of an electron is $-e$ .
9-50 (8-44)	charge number of ion <i>fr nombre (m) de charge d'un ion, électrovalence (f)</i>	$z$	ratio of the electric charge (IEC 80000-6:2008, item 6-2) of the ion to the elementary charge (item 9-49)	
9-51 (8-45)	Faraday constant <i>fr constante (f) de Faraday</i>	$F$	$F = N_A e$ where $N_A$ is the Avogadro constant (item 9-4) and $e$ is the elementary charge (item 9-49)	$F = 96,485\ 339\ 9(24) \times 10^3\ \text{C/mol}$ [CODATA 2006]
9-52 (8-46)	ionic strength <i>fr force (f) ionique</i>	$I$	$I = \frac{1}{2} \sum z_i^2 b_i$ where the summation is carried out over all ions with charge number $z_i$ (item 9-50) and molality $m_i$ (item 9-16)	
9-53 (8-47)	degree of dissociation <i>fr facteur (m) de dissociation</i>	$\alpha$	ratio of the number of dissociated molecules to the total number of molecules	An alternative name for this quantity is "dissociation fraction".
9-54 (8-48)	electrolytic conductivity <i>fr conductivité (f) électrolytique</i>	$\varkappa, \sigma$	$\varkappa = J/E$ where $J$ is the electrolytic current density (IEC 80000-6:2008, item 6-8) and $E$ is the electric field strength (IEC 80000-6:2008, item 6-10)	
9-55 (8-49)	molar conductivity <i>fr conductivité (f) molaire</i>	$\Lambda_m$	$\Lambda_m = \varkappa/c_B$ where $\varkappa$ is the electrolytic conductivity (item 9-54) and $c_B$ is the amount-of-substance concentration (item 9-13)	

UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-49.a	coulomb	C		
9-50.a	one	1		See the Introduction, 0.3.2.
9-51.a	coulomb per mole	C/mol		
9-52.a	mole per kilogram	mol/kg		
9-53.a	one	1		See the Introduction, 0.3.2.
9-54.a	siemens per metre	S/m		
9-55.a	siemens metre squared per mole	S · m <sup>2</sup> /mol		

(continued)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	Name	Symbol	Definition	Remarks
9-56 (8-50)	transport number of the ion B, current fraction of the ion B <i>fr nombre (m) de transport du constituant ionique B</i>	$t_B$	$t_B = i_B/i$ where $i_B$ is the electric current (IEC 80000-6:2008, item 6-1) carried by the ion B and $i$ is the total electric current	
9-57 (8-51)	angle of optical rotation <i>fr angle (m) de rotation optique</i>	$\alpha$	angle through which plane-polarized light is rotated clockwise, as seen when facing the light source, in passing through an optically active medium	
9-58 (8-52)	molar optical rotatory power <i>fr rotation (f) spécifique molaire</i>	$\alpha_n$	$\alpha_n = \alpha A/n$ where $\alpha$ is the angle of optical rotation (item 9-57), and $n$ is the amount of substance (item 9-1) of the optically active component in the path of a linearly polarized light beam of cross-sectional area (ISO 80000-3:2006, item 3-3) $A$	
9-59 (8-53)	specific optical rotatory power <i>fr rotation (f) spécifique massique</i>	$\alpha_m$	$\alpha_m = \alpha A/m$ where $\alpha$ is the angle of optical rotation (item 9-57), and $m$ is the mass (ISO 80000-4:2006, item 4-1) of the optically active component in the path of a linearly polarized light beam of cross-sectional area (ISO 80000-3:2006, item 3-3) $A$	



UNITS		PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS		
Item No.	Name	Inter-national symbol	Definition	Conversion factors and remarks
9-56.a	one	1		See the Introduction, 0.3.2.
9-57.a	radian	rad		
9-58.a	radian square metre per mole	rad · m <sup>2</sup> /mol		See the Introduction, 0.3.2.
9-59.a	radian square metre per kilogram	rad · m <sup>2</sup> /kg		

(end)

## Annex A (normative)

### Atomic numbers, names, and symbols for the chemical elements

Atomic number	Name	Symbol	Atomic number	Name	Symbol
1	hydrogen	H	35	bromine	Br
2	helium	He	36	krypton	Kr
3	lithium	Li	37	rubidium	Rb
4	beryllium	Be	38	strontium	Sr
5	boron	B	39	yttrium	Y
6	carbon	C	40	zirconium	Zr
7	nitrogen	N	41	niobium	Nb
8	oxygen	O	42	molybdenum	Mo
9	fluorine	F	43	technetium	Tc
10	neon	Ne	44	ruthenium	Ru
11	sodium, (natrium)	Na	45	rhodium	Rh
12	magnesium	Mg	46	palladium	Pd
13	aluminium	Al	47	silver, (argentum)	Ag
14	silicon	Si	48	cadmium	Cd
15	phosphorus	P	49	indium	In
16	sulfur	S	50	tin, (stannum)	Sn
17	chlorine	Cl	51	antimony, (stibium)	Sb
18	argon	Ar	52	tellurium	Te
19	potassium, (kalium)	K	53	iodine	I
20	calcium	Ca	54	xenon	Xe
21	scandium	Sc	55	caesium	Cs
22	titanium	Ti	56	barium	Ba
23	vanadium	V	57	lanthanum	La
24	chromium	Cr	58	cerium	Ce
25	manganese	Mn	59	praseodymium	Pr
26	iron, (ferrum)	Fe	60	neodymium	Nd
27	cobalt	Co	61	promethium	Pm
28	nickel	Ni	62	samarium	Sm
29	copper, (cuprum)	Cu	63	europium	Eu
30	zinc	Zn	64	gadolinium	Gd
31	gallium	Ga	65	terbium	Tb
32	germanium	Ge	66	dysprosium	Dy
33	arsenic	As	67	holmium	Ho
34	selenium	Se	68	erbium	Er

Atomic number	Name	Symbol
69	thulium	Tm
70	ytterbium	Yb
71	lutetium	Lu
72	hafnium	Hf
73	tantalum	Ta
74	tungsten, (wolfram)	W
75	rhenium	Re
76	osmium	Os
77	iridium	Ir
78	platinum	Pt
79	gold, (aurum)	Au
80	mercury, (hydrargyrum)	Hg
81	thallium	Tl
82	lead, (plumbum)	Pb
83	bismuth	Bi
84	polonium	Po
85	astatine	At
86	radon	Rn
87	francium	Fr
88	radium	Ra
89	actinium	Ac
90	thorium	Th
91	protactinium	Pa
92	uranium	U
93	neptunium	Np
94	plutonium	Pu

Atomic number	Name	Symbol
95	americium	Am
96	curium	Cm
97	berkelium	Bk
98	californium	Cf
99	einsteinium	Es
100	fermium	Fm
101	mendelevium	Md
102	nobelium	No
103	lawrencium	Lr
104	rutherfordium	Rf
105	dubnium	Db
106	seaborgium	Sg
107	bohrium	Bh
108	hassium	Hs
109	meitnerium	Mt
110	darmstadtium	Ds
111	röntgenium (roentgenium)	Rg

NOTE 1 IUPAC spells the chemical element 111 "roentgenium" in English. ISO/TC 12 considers that is wrong, because the name is derived from the first Nobel (compare the chemical element 102) prize winner in physics 1901, Wilhelm Konrad Röntgen, DE. Compare also <sup>A1</sup>ISO 80000-10:2009, item 10-92.a<sup>A1</sup>, where the unit is röntgen, symbol R ( $1 \text{ R} = 2,58 \times 10^{-4} \text{ C/kg}$ ). Compare also the unit ångström, symbol Å, ( $1 \text{ Å} = 10^{-10} \text{ m}$ ) after Anders Ångström, SE. Both of these names and symbols with German and Swedish letters are adopted by CIPM.

NOTE 2 The names in parentheses are added for information.

**A1** Annex B  
(normative)

## Symbols for chemical elements and nuclides

Symbols for chemical elements shall be written in roman (upright) font with a capital initial and often followed by one lower case letter. The symbol is not followed by a full stop except at the end of a sentence.

### EXAMPLES

H As Th

The attached subscripts and superscripts specifying a nuclide or molecule shall have the following meanings and positions, all physical notations being on the left of the symbol and all chemical notations being on the right.

The nucleon number (mass number) of a nuclide is shown in the left superscript position, as in the following example.

$^{14}\text{N}$

The number of atoms of a nuclide in a molecule is shown in the right subscript position, as in the following example.

$^{14}\text{N}_2$

The atomic number (proton number) is shown in the left subscript position, as in the following example.

$_{64}\text{Gd}$

The state of ionization is shown in the right superscript position, as in the following examples.

$\text{Na}^+$ ,  $\text{PO}_4^{3-}$ ,  $(\text{PO}_4)^{3-}$

The state of electrical excitation is shown in the right superscript position, as in the following examples.

$\text{He}^*$ ,  $\text{NO}^*$

The state of nuclear excitation is shown with the symbol \* in the left superscript position and for a metastable nuclide is indicated by adding the letter m (in roman type) to the mass number of the nuclide, as in the following example.

$^{137*}\text{Xe}$ , or when metastable,  $^{133\text{m}}\text{Xe}$  **A1**

## Annex C (normative)

### pH

The following definition of pH is quoted from the IUPAC Green Book, *Quantities, Units and Symbols in Physical Chemistry*, 3rd ed., 2007<sup>[4]</sup>, with permission from IUPAC.

The quantity pH is defined in terms of the activity of hydrogen (1+) ions (hydrogen ions) in solution:

$$\text{pH} = \text{p}a_{\text{H}^+} = -\lg(a_{\text{H}^+}) = -\lg(m_{\text{H}^+} \gamma_{\text{m,H}^+} / m^{\ominus})$$

where  $a_{\text{H}^+}$  is the activity of the hydrogen (1+) (hydrogen ion) in solution,  $\text{H}^+$  (aq), and  $\gamma_{\text{m,H}^+}$  is the activity coefficient of  $\text{H}^+$  (aq) on the molality basis at molality  $m_{\text{H}^+}$ .

The symbol p is interpreted as an operator ( $\text{p}x = -\lg x$ ) with the unique exception of the symbol pH. The symbol pH is also an exception to the rules for symbols and quantities. The standard molality  $m^{\ominus}$  is chosen to be equal to  $1 \text{ mol} \cdot \text{kg}^{-1}$ . Since pH is defined in terms of a quantity that cannot be measured independently, the above equation can only be regarded as a *notional* definition.

The establishment of primary pH standards requires the application of the concept of the “primary method of measurement”, ensuring full traceability of the results of all measurements and their uncertainties. Any limitation in the theory or determination of experimental variables shall be included in the estimated uncertainty of the method.

The primary method for the measurement of pH involves the use of a cell without transference, known as the *Harned cell*:



Application of the Nernst equation to the above leads to the relationship

$$E = E^{\ominus} - \frac{RT \ln 10}{F} \lg \left[ (m_{\text{H}^+} \gamma_{\text{H}^+} / m^{\ominus}) (m_{\text{Cl}^-} \gamma_{\text{Cl}^-} / m^{\ominus}) \right]$$

where  $E$  is the potential difference of the cell and  $E^{\ominus}$  the standard potential of the  $\text{AgCl} \mid \text{Ag}$  electrode. This equation can be rearranged to yield

$$-\lg(a_{\text{H}^+} \gamma_{\text{Cl}^-}) = \frac{E - E^{\ominus}}{(RT \ln 10) / F} + \lg(m_{\text{Cl}^-} / m^{\ominus})$$

Measurements of  $E$  are made and the quantity  $-\lg(a_{\text{H}^+} \gamma_{\text{Cl}^-})$  is obtained by extrapolation to  $m_{\text{Cl}^-} / m^{\ominus} = 0$ . The value of  $\gamma_{\text{Cl}^-}$  is calculated using the Bates-Guggenheim convention based on Debye-Hückel theory. Then  $-\lg(a_{\text{H}^+})$  is calculated and identified as pH(PS), where PS signifies primary standard. The uncertainties in the two estimates are typically  $\pm 0,001$  in  $-\lg(a_{\text{H}^+} \gamma_{\text{Cl}^-})^{\ominus}$  and  $\pm 0,003$  in pH.

Materials for primary standard pH buffers shall also meet the appropriate requirements for reference materials, including chemical purity and stability, and applicability of the Bates-Guggenheim convention to the estimation of  $-\lg(\gamma_{\text{Cl}^-})$ . This convention requires that the ionic strength be  $\leq 0,1 \text{ mol} \cdot \text{kg}^{-1}$ . Primary standard buffers should also lead to small liquid junction potentials when used in cells with liquid junctions. Secondary standards, pH(SS), are also available, but carry a greater uncertainty in measured values.

Practical pH measurements generally use cells involving liquid junctions in which, consequently, liquid junction potentials,  $E_j$ , are present. Measurements of pH are not normally performed using the Pt | H<sub>2</sub> electrode, but rather the glass (or another H<sup>+</sup>-selective) electrode, whose response factor ( $dE/dpH$ ) usually deviates from the Nernst slope. The associated uncertainties are significantly larger than those associated with the fundamental measurements using the Harned cell. Nonetheless, incorporation of the uncertainties for the primary method, and for all subsequent measurements, permits the uncertainties for all procedures to be linked to the primary standards by an unbroken chain of comparisons.

Reference values for standards in D<sub>2</sub>O and aqueous-organic solvent mixtures exist.

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- [A1] [1] ISO 80000-1:2009, *Quantities and units — Part 1: General*
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- [3] CODATA 2006, <http://physics.nist.gov/cuu/Constants/bibliography.html>
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